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소성변형의 분자론 (제 1 보). 이론

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Molecular Theory of Plastic Deformation (I). Theory

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요 약. 고체의 소성변형을 설명하기 위하여 다음과 같은 가정을 하였다.

(1) 고체의 소성변형은 크게 두 가지 기구 즉 dislocation 운동과 grain boundary 운동에 의하여 일어난다. (2) Dislocation 운동에 있어서 유동 단위들은 역학적 모형으로 나타내면 다종의 Maxwell 단위들의 평행연결형으로 되고 grain boundary 유동단위들도 다종의 Maxwell 단위들의 평행연결로 표현된다. 이를 물리적으로 설명하면 같은 부류의 유동단위들은 모두 같은 shear plane 에서 같은 shear rate 로 흐름을 의미한다. (3) Grain boundary 유동단위들과 dislocation 유동단위들 같은 서로 직렬 연결되어 있다. 이는 물리적으로 고체내에서 stress 는 균일하게 작용하나 shear rate 는 shear plane 의 종류(dislocation 운동면과 grain boundary 운동면)에 따라 달리 나타남을 의미한다. (4) Dislocation 유동단위들과 grain boundary 운동단위들의 운동은 그들의 흐름을 방해하는 장애물 근방의 원자 또는 분자들이 확산해 나가므로써 가능하게 된다.

이러한 가정하에 반응속도론을 적용하여 shear rate 와 shear stress 를 구하는 일반식을 도출하였다. 본 연구에서는 실제로 중요한 네가지 경우에 대하여 상기 도출한 일반식을 고찰하였다.

ABSTRACT. In order to elucidate the plastic deformation of solids, the following assumptions were made: (1) the plastic deformation of solids is classified into two main types, the one which is caused by dislocation movement and the other caused by grain boundary movement, each movement being restricted on a different shear surface, (2) the dislocation movement is expressed by a mechanical model of a parallel connection of various kinds of Maxwell dislocation flow units whereas the grain boundary movement is also expressed by a parallel connection of various kinds of Maxwell grain boundary flow units; the parallel connection in each type of movements indicates that all the flow units on each shear surface flow with the same shear rate, (3) the latter model for grain boundary movement is connected in series to the former for dislocation movement, this means physically that the applied stress distributes homogeneously in the flow system while the total strain rate distributes heterogeneously on the two types of shear planes (dislocation or grain boundary shear plane), (4) the movement of dislocation flow units and grain boundary units becomes possible when the atoms or molecules near the obstacles, which hinder the movement of flow units, diffuse away from the obstacles.

Using the above assumptions in conjunction with the theory of rate processes, generalized equations of shear stress and shear rate for plastic deformation were derived. In this paper, four cases important in practice were considered.

INTRODUCTION

Many theories of plastic deformation of solids have been proposed. The Nabarro-Herring theory[1] of lattice diffusion and Coble's grain boundary diffusion theory[2] are the representatives. The above-mentioned theories were intensively studied by Folweiler,[3] Warshaw and Norton,[4] Kingery and Montrone,[5] and compared with experiment, but the results were not so successful.

On the other hand the Ree-Eyring theory, based on the theory of rate processes, was successful in a wide range of applications in elucidating the plastic deformations of polymeric solutions[6] and melts,[7] alloys,[8] and Yule marble.[9] The results are presented in Ree and Eyring's review articles[10,11] and in Krausz and Eyring's recent book[12] in detail.

Of the articles mentioned above, reference 9 is concerned with the deformation of Yule marble. Here, Hahn, Ree and Eyring proposed the theory that the deformation is explained by a model of series connection of a single kind of dislocation Maxwell units and another single kind of grain boundary Maxwell units. The Hahn-Ree-Eyring(HRE) theory was very successfully applied to the Yule marble deformation. In this paper the HRE thory is more refined and extended to make it applicable for various experimental cases.

THEORY

According to Ree-Ree-Eyring theory,[6~8] plastic deformation of metals and alloys occurs by dislocation movement, and the relationships between stress and strain rate are expressed as follows:

$$f_d=\sum_{i=1}^{n}\frac{X_{di}}{\alpha_{di}}\sinh^{-1}(\beta_{di}\,\dot{s}_d). \tag{1a}$$

$$\dot{s}_d=\dot{s}_{d1}=\dot{s}_{d2}\cdots\cdots=\dot{s}_{di}=\cdots\cdots \tag{1b}$$

$$\dot{s}_d=\left(\frac{\lambda}{\lambda_1}2k'\right)_{di}\sinh\left[\left(\frac{\lambda\lambda_2\lambda_3}{2kT}\right)_{di}f_{di}\right]$$
$$\equiv(\beta_{di})^{-1}\sinh(\alpha_{di}f_{di}) \tag{1c}$$

$$\alpha_{di}\equiv\left(\frac{\lambda\lambda_2\lambda_3}{2kT}\right)_{di} \tag{1d}$$

$$(\beta_{di})^{-1}\equiv\left(\frac{\lambda}{\lambda_1}2k'\right)_{di} \tag{1e}$$

Here the subscript d represents dislocation, f_d the total stress applied on a dislocation slip plane, $\dot{s}_d$ the total strain rate of the dislocation movement, $1/\alpha_{di}$ and $1/\beta_{di}$ are[8] the intrinsic shear stress and intrinsic shear rate of the ith kind of dislocation flow units, respectively, X_{di} the fraction of the area occupied by the ith kind of dislocation flow units on the dislocation slip plane, k' is the jump frequency of the flow unit from an equilibrium position to the next equilibrium position when stress is zero, λ is the distance between two successive equilibrium positions, and λ_1, λ_2, λ_3 are the molecular parameters of Eyring's flow theory.[13] In the above equations, the subscript di outside the parentheses indicates that the inside quantities of the parentheses belong to the ith dislocation flow unit.

Physically Eq. (1b) signifies that all the dislocation flow units on a slip plane flow with the same shear rate. The mechanical model corresponding to Eq. (1b) is shown in *Fig.* 1a where various Maxwell units differing in relaxation time τ (proportional to β) are connected in parallel. The stress f_{di} on flow unit (di) is equal to f_{dm} if $\tau_{di}=\tau_{dm}$, otherwise $f_{di}\neq f_{dm}$.

In the Ree-Ree-Eyring theory[8] the plastic deformation was considered to occur only by

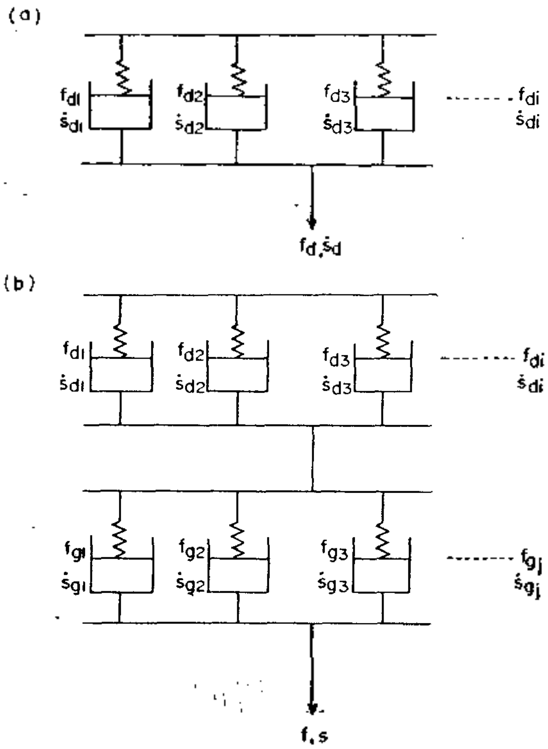

Fig. 1. Mechanical models illustrating the deformation mechanisms. (a) Parallel combination of Maxwell dislocaton flow units. (b) Series combination of two systems, one of which is the parallel combination of Maxwell dislocation flow units, and the other is the parallel combination of Maxwell grain boundary flow units.

the dislocation movement on a dislocation shear plane. But in actual polycrystalline solids, there are many grain boundaries, and plastic deformation caused by the grain boundary movement has been experimentally proved.[14] By a similar reasoning as in the case for the dislocation movement, the grain boundary movement is also represented by a similar model as shown in *Fig.* 1a where all the subscript d is replaced by the subscript g representing the grain boundary. Thus, the following equations corresponding to Eqs. (1a), (1b) and (1c) hold for the grain boundary movement:

$$f_g = \sum_j \frac{X_{gj}}{\alpha_{gj}} \sinh^{-1}(\beta_{gj}\dot{s}_g) \tag{2a}$$

$$\dot{s}_g = \dot{s}_{g1} = \dot{s}_{g2} = \cdots\cdots = \dot{s}_{gj} = \cdots\cdots \tag{2b}$$

and

$$\dot{s}_g = \left(\frac{\lambda}{\lambda_1} 2k'\right)_{gj} \sinh\left[\left(\frac{\lambda\lambda_2\lambda_3}{2kT}\right)_{gj} f_{gj}\right] \equiv (\beta_{gj})^{-1}\sinh(\alpha_{gj} f_{gj}) \tag{2c}$$

Now, it is appropriate to consider the contributions of stresses f_d and f_g to total stress f, and the contributions of strain rates $\dot{s}_d$ and $\dot{s}_g$ to total strain rate $\dot{s}$. When stress is applied to a solid, the stress is homogeneously distributed throughout the flow system. Thus it is considered that the applied shear stresses on the dislocation and grain boundary slip planes are the same. And from the structural point of view, it is clear that dislocation slip planes are located within the grain, and that grain boundaries are the regions where the concentration of vacancies is high and atoms are fairly randomly distributed. Thus it is assumed that there are two types of independent slip planes in the polycrystals, i. e., the dislocation slip planes within the grain and the slip plane on the grain boundary. When stress is applied to a flow system, the magnitudes of shear stress on both types of shear planes are the same, whereas the shear rates on each shear plane are different, the total shear rate being expressed as the sum of shear rates on the different types of shear planes. This concept corresponds to a mechanical model shown in *Fig.* 1b. One notes from *Fig.* 1b that this model is consisted of two parts, one representing the dislocation movement and the other representing the grain boundary movement, the two parts being connected in series. One also notes that the former part is exactly equal to the model represented by *Fig.* 1a for dislocation movement while the latter part is very similar to *Fig.* 1a in which all the subscript d were replaced by the subscript g representing the grain boundary movement. With the above–

mentioned mechanical model, total strain rate $\dot{s}$ can be expressed by the following equation:

$$\dot{s} = \dot{s}_d + \dot{s}_g \tag{3}$$

and the total stress f becomes

$$f = f_d = \sum_i X_{di} f_{di} = f_g = \sum_j X_{gj} f_{gj} \tag{4}$$

Introducing Eqs. (1c) and (2c) into Eq. (3), one obtains

$$\dot{s} = \frac{1}{\beta_{di}} \sinh\left(\frac{\alpha_{di}}{X_{di}} X_{di} f_{di}\right) + \frac{1}{\beta_{gj}} \sinh\left(\frac{\alpha_{gj}}{X_{gj}} X_{gj} f_{gj}\right) \tag{5}$$

In Eq. (5) $X_{di} f_{di}$, $X_{gj} f_{gj}$ are the quantities that can be determined from the observed values of $\dot{s}$ and f after some analysis. Now, Eqs. (4) and (5) are considered as the generalized equations for plastic deformations of polycrystalline solids since by various combinations of flow units di, gj many types of plastic deformation patterns would be produced. In the following, four cases which are important in practice will be considered.

CALCULATIONS OF FLOW CURVES

Case 1. This is the case where only one kind of flow units are acting. For the deformation due to dislocation movement, the following equations are immediately derived from Eqs. (4) and (5):

$$\left.\begin{aligned} f &= f_d = X_{d1} f_{d1} = f_{d1} \\ \dot{s} &= \frac{1}{\beta_{d1}} \sinh\left(\frac{\alpha_{d1}}{X_{d1}} X_{d1} f_{d1}\right) \\ &= \frac{1}{\beta_{d1}} \sinh(\alpha_{d1} f) \end{aligned}\right\} \tag{6a}$$

Similarly, the following equations are derived for grain boundary movement:

$$\left.\begin{aligned} f &= f_g = X_{g1} f_{g1} = f_{g1} \\ \dot{s} &= \frac{1}{\beta_{g1}} \sinh\left(\frac{\alpha_{g1}}{X_{g1}} X_{g1} f_{g1}\right) \\ &= \frac{1}{\beta_{g1}} \sinh(\alpha_{g1} f) \end{aligned}\right\} \tag{6b}$$

Here, Eq. (6a) applies to the deformation of single crystals. One will notice that the grain boundary sliding would occur at a lower stress level than that of dislocation motion because of the presence of many vacancies in the grain boundaries which act also sinks of vacancies.

Case 2. Next, we consider the case where all the flow units are connected in parallel. For this pattern, two cases are possible, in one of which all units are dislocation flow units, and in the other all are grain boundary flow units. For these cases Eqs. (4) and (5) are transformed into the following equations:

$$\left.\begin{aligned} f &= \sum_i^m X_{di} f_{di} \\ \dot{s} &= \frac{1}{\beta_{di}} \sinh\left(\frac{\alpha_{di}}{X_{di}} X_{di} f_{di}\right) \end{aligned}\right\} \tag{7a}$$

or

$$\left.\begin{aligned} f &= \sum_j^m X_{gj} f_{gj} \\ \dot{s} &= \frac{1}{\beta_{gj}} \sinh\left(\frac{\alpha_{gj}}{X_{gj}} X_{gj} f_{gj}\right) \end{aligned}\right\} \tag{7b}$$

The plot of f *vs.* $-ln\ \dot{s}$ for Eq. (7b) is visualized schematically in *Fig.* 2a, where by convenience a parallel connection of two kinds of grain boundary flow units is considered. In *Fig.* 2a, the broken line GB1 indicates the curve for grain boundary flow units 1, broken line GB2 for flow units 2, and the solid line is the curve synthesized from GB1 and GB2. The contribution of the stress by GB2 to the total stress (full curve) is predominant at the low stress level where that by GB1 is negligible, i.e., the flow behavior of the solid is nearly equal to that of GB2. Thus, the flow parameters of GB2 (α_{g2}/X_{g2} and $1/\beta_{g2}$) can be easily obtained in this region (for the method refer to Case 3). When the stress level is high, however, the two contributions are comparable, and by performing the processes (3), (4) and (5) in Appendix 1, the parameters, α_{g1}/X_{g1} and $1/\beta_{g1}$

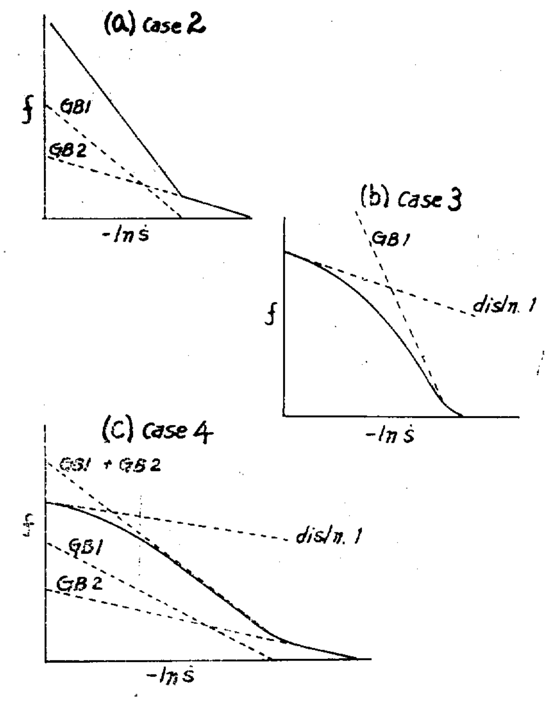

Fig. 2. Schematic representation of flow curves of f *vs.* $-\ln \dot{s}$. (a) Case 2: two kinds of grain boundary flow units are connected in parallel. (b) Case 3: one kind of grain boundary flow units is connected in series with one kind of dislocation flow units. (c) Case 4: one kind of dislocation flow units is connected in series with a system in which two kinds of grain boundary flow units are connected in parallel.

can be obtained. Thus, the curve of f *vs.* $-\ln \dot{s}$ is calculated by using the following equation:

$$f=\frac{X_{g1}}{\alpha_{g1}}\sinh^{-1}\beta_{g1}\dot{s}+\frac{X_{g2}}{\alpha_{g2}}\sinh^{-1}\beta_{g2}\dot{s} \quad (7c)$$

which is obtained by introducing the relation of f *vs.* $\dot{s}$ obtained from the second equation of Eq. (7b) to the first equation where $m=2$.

The above-mentioned analysis can be applied to the case of dislocation movement, which is similar to the above case, and which occurs in single crystal systems.

Case 3. Next, let us consider the case where a single kind of dislocation flow units and another single kind of grain boundary flow units are connected in series. Eqs. (4) and (5) are transformed into the following equations:

$$f=f_d=X_{d1}f_{d1}=f_{d1}=f_g=X_{g1}f_{g1}=f_{g1} \quad (8)$$

$$\dot{s}=\frac{1}{\beta_{d1}}\sinh\left(\frac{\alpha_{d1}}{X_{d1}}X_{d1}f_{d1}\right)+\frac{1}{\beta_{g1}}\sinh\left(\frac{\alpha_{g1}}{X_{g1}}X_{g1}f_{g1}\right)=\frac{1}{\beta_{d1}}\sinh(\alpha_{d1}f)+\frac{1}{\beta_{g1}}\sinh(\alpha_{g1}f) \quad (9)$$

The schematic plot f *vs.* $-\ln \dot{s}$ for Eq. (9) is shown in *Fig.* 2b. In *Fig.* 2b the broken line, disln. 1, denotes the part contributed by the flow units of dislocation movement, the broken line, GB1, indicates the part contributed by those of grain boundary movement, and the solid line is the synthesized curve from disln. 1 and GB1. In the high stress level, the strain rate of disln. 1 is approximately equal to the total strain rate $\dot{s}$, and the contribution of GB1 to the total $\dot{s}$ is negligible*. On the other hand, in the low stress level, the contribution of GB1 to the total strain rate is predominant while that of disln. 1 is negligible. Generally, the system, for which the above-mentioned approximation is applicable, can be treated as a plastic deformation system composed of only a single type of flow units in the extreme stress ranges. That is, in the stress range, where the mechanism kn ($kn=di$ or gj) contributes predominantly, $\dot{s}$ can be approximated by Eq. (10),

$$\dot{s}\cong\frac{1}{\beta_{kn}}\sinh\left(\frac{\alpha_{kn}}{X_{kn}}X_{kn}f_{kn}\right)\cong\frac{1}{\beta_{kn}}\sinh\left(\frac{\alpha_{kn}}{X_{kn}}f\right) \quad (10)$$

Differentiation of Eq. (10) yields

* This fact is not immediately clear from *Fig.* 2*b*, this is due to the fact that the abscissa is $-\ln \dot{s}$. If *Fig.* 2b is represented by the plot of f *vs.* $\dot{s}$, the negligible contribution of GB1 to $\dot{s}$ will be clearer.

$$\frac{df}{d\ln\dot{s}} = \frac{X_{kn}}{\alpha_{kn}}\tanh\left(\frac{\alpha_{kn}}{X_{kn}}f\right) \cong \frac{X_{kn}}{\alpha_{kn}} \quad (11)$$

If $(\alpha_{kn}/X_{kn})f \geq 2$, then the second approximate equality of Eq. (11) holds. Eq. (11) represents a slope in the curve of f *vs.* In $\dot{s}$. Thus the parameter α_{kn}/X_{kn} can be easily obtained from the slope of the curve. Introducing the value of α_{kn}/X_{kn} into Eq. (10), and using experimental data $\dot{s}$. and f, the quantity $1/\beta_{kn}$ can be evaluated.

Case 4. Now let us consider the fourth case where one kind of dislocation flow units is connected in series with a system in which two kinds of grain boundary flow units are connected in parallel. In this case, Eqs. (4) and (5) can be transformed into:

$$f = f_d = X_{d1}f_{d1} = f_{d1} = f_g = X_{g1}f_{g1} + X_{g2}f_{g2} \quad (12)$$

$$\begin{aligned}\dot{s} &= \frac{1}{\beta_{d1}}\sinh\left(\frac{\alpha_{d1}}{X_{d1}}X_{d1}f_{d1}\right) + \frac{1}{\beta_{g2}}\sinh\frac{\alpha_{g2}}{X_{g2}}X_{g2}f_{g2}\Big) \\ &= \frac{1}{\beta_{d1}}\sinh(\alpha_{d1}f) + \frac{1}{\beta_{g2}}\sinh\frac{\alpha_{g2}}{X_{g2}}X_{g2}f_{g2}\Big) \quad (13)\end{aligned}$$

The schematic plot f *vs.* $-\ln\dot{s}$ for Eqs. (12) and (13) are shown in ***Fig.*** 2c. In ***Fig.*** 2c, the broken lines GB1 and GB2 indicate the curve for the grain boundary flow units 1 and 2, respectively, the broken line (GB1+GB2) represents the synthesized curve from GB1 and GB2, the broken line disln. 1 indicates the contribution of the dislocation flow units, and the solid line is for the result of synthesis from the curves (GB1+GB2) and disln. 1. Now let us examine the contributions by each types of flow units to the total strain rate in the high stress region. Here the contribution by disln. 1 is predominant while that by (GB1+GB2) is negligible. However, the reverse is true over the low stress region. Furthermore, in this region, one finds that the contribution of GB1 to the total stress f in a very small $\dot{s}$ region is negligible compared to GB2. Accordingly, over the two extreme stress ranges where the above mentioned approximations are applicable, the plastic deformation in each stress region can be described by a single type of flow units. Thus, by using the Eqs. (10) and (11), one can calculate the flow parameters $(\alpha_{d1}, 1/\beta_{d1})$ and $(\alpha_{g2}/X_{g2}, 1/\beta_{g2})$. The contribution by GB1 is considerable in the middle range of stress. The determination of parameters α_{g1}/X_{g1} and $1/\beta_{g1}$ is carried out by a little lengthy manupulation as described in Appendix 1.

According to Eq. (13), total strain rate $\dot{s}$ can be calculated at a given stress f with the parameters α_{d1}, $1/\beta_{d1}$, α_{g2}/X_{g2} and $1/\beta_{g2}$ provided that the value $X_{g2}f_{g2}$ be known. The quantity $X_{g2}f_{g2}$ can be calculated by the following method. Since $\dot{s}_{g1} = \dot{s}_{g2}$, one obtains the following relationship,

$$\begin{aligned}&\frac{1}{\beta_{g1}}\sinh\left(\frac{\alpha_{g1}}{X_{g1}}X_{g1}f_{g1}\right) \\ &= \frac{1}{\beta_{g2}}\sinh\left(\frac{\alpha_{g2}}{X_{g2}}X_{g2}f_{g2}\right) \\ &= \frac{1}{\beta_{g1}}\sinh\left[\frac{\alpha_{g1}}{X_{g1}}(f - X_{g2}f_{g2})\right]\end{aligned}$$

where the relation $f = X_{g1}f_{g1} + X_{g2}f_{g2}$ [Eq. (12)] has been applied. Rearranging this equation yields Eq. (14),

$$\frac{\sinh\left[\frac{\alpha_{g1}}{X_{g1}}(f - X_{g2}f_{g2})\right]}{\sinh\left(\frac{\alpha_{g2}}{X_{g2}}X_{g2}f_{g2}\right)} = \frac{\beta_{g1}}{\beta_{g2}} \equiv c \quad (14)$$

where constant c can be obtained from the previously determined values of $1/\beta_{g1}$ and $1/\beta_{g2}$. From Eq. (14), the quantity, $X_{g2}f_{g2}$, is calculated at a given stress f. Consequently, the curve of f *vs.* $-\ln\dot{s}$ is theoretically calculated from Eq. (13).

CALCULATIONS OF ACTIVATION ENTHALPIES

According to Eyring's theory,[13] k' in Eq. (1e) can be rewritten

$$k'=\frac{kT}{h}\exp\frac{\Delta S^{\neq}}{R}\cdot\exp\left(-\frac{\Delta H^{\neq}}{RT}\right)$$

Introducing this relation to Eq. (1e), one obtains the following equation:

$$\frac{1}{\beta_{di}}=(\dot{s}_{di})_0\exp-\left(\frac{\Delta H^{\neq}_{di}}{RT}\right) \quad (15a)$$

and similarly,

$$\frac{1}{\beta_{gj}}=(\dot{s}_{gj})_0\exp\left(-\frac{\Delta H^{\neq}_{gj}}{RT}\right) \quad (15b)$$

where

$$(\dot{s}_{di})_0=\left\{\frac{\lambda}{\lambda_1}\,\frac{2kT}{h}\exp\left(\frac{\Delta S^{\neq}}{R}\right)\right\}_{di} \quad (15c)$$

and

$$(\dot{s}_{gj})_0=\left\{\frac{\lambda}{\lambda_1}\,\frac{2kT}{h}\exp\left(\frac{\Delta S^{\neq}}{R}\right)\right\}_{gj} \quad (15d)$$

The quantities $(\dot{s}_{di})_0$ and $(\dot{s}_{gj})_0$ can be treated as temperature independent quantities. Introducing $\beta_{kn}(kn=di$ or $gj)$ into Eq. (1c) or (2c), one obtains

$$\dot{s}_k=(\dot{s}_{kn})_0\exp\left(-\frac{\Delta H^{\neq}_{kn}}{RT}\right)\sinh(\alpha f)_{kn} \quad (16a)$$

From Eq. (16a), the following equation for activation enthalpy $\Delta H^{\neq}_{kn}$ is derived:

$$\Delta H^{\neq}_{kn}=-\frac{RT_1T_2}{T_2-T_1}\ln\frac{\dot{s}^{(1)}}{\dot{s}^{(2)}} \quad (16b)$$

where $\dot{s}^{(1)}$ and $\dot{s}^{(2)}$ are, respectively, the strain rates at temperatures T_1 and T_2 at a given stress f, and both are given by Eq. (16a) where α_{kn} is a temperature independent quantity[8].

The substitution of Eq. (15a) and (15b) into Eq. (9) for Case 3 yields,

$$\dot{s}=(\dot{s}_{d1})_0\exp\left(-\frac{\Delta H^{\neq}_{d1}}{RT}\right)\sinh(\alpha_{d1}f)$$
$$+(\dot{s}_{g1})_0\exp\left(-\frac{\Delta H^{\neq}_{g1}}{RT}\right)\sinh(\alpha_{g1}f) \quad (17)$$

When $\Delta H^{\neq}_{g1}$ and $1/\beta_{g1}$ are known, $(\dot{s}_{g1})_0$ can be calculated by the use of Eq. (15b). If one assume $(\dot{s}_{d1})_0=(\dot{s}_{g1})_0$ in Eq. (17), $\Delta H^{\neq}_{d1}$ can easily be determined by using the experimental data $\dot{s}$ and f at a given temperature in conjunction with α_{d1} and α_{g1} which were determined previously. This indirect method is employed when $\Delta H^{\neq}_{d1}$ is not able to calculate from Eq. (16) because of the lack of experimental data.

DISCUSSIONS

(1) Molecular View of the Deformation Mechanisms. It is well known that the velocity of a dislocation line on a slip plane is very fast when there are no obstacles during slip.[15] But actually there are many obstacles (bad sites) on the slip plane as well as on the dislocation line such as impurities, alloying elements, and lattice defects. Whenever the bad site on the dislocation line encounters the bad site on the slip plane, the movement of the line is held up; as a result, the held-up flow unit concentrates stress on the atoms neighboring the obstacles on the slip plane. The stress is relieved when the neighboring atoms move away from the obstacles on the slip plane by self-diffusion, and then the held-up dislocation line can move forward. From this point of view, Ree-Ree-Eyring theory[8] treated the dislocation movement by using the theory of rate processes.[13] Here the dislocation-line bad sites are considered to be the flow units.

Next, we consider the grain boundary movements. There are also many obstacles (or bad sites) on the surface of grain boundaries such as ledges,[16] bumps,[17] precipitates,[18a] grain boundary dislocations,[18b] and impurities,[18a] and these bad sites are considered to impede the shear of the two grains in contact. When a bad site (flow unit) on the boundary surface of grain A encounters a bad site on the grain boundary slip plane of grain B, the former applies a high stress on the latter. To relieve this high stress, atoms near the latter move away by self-diffusion. After enough self-diffusion, the bad sites of grain A can pass the bad sites of grain B. So the process of self-diffusion is considered to be the rate-determining step of the slip rate (or shear rate). There are many kinds of flow units on a shear surface, but they flow with the same shear rate $\dot{s}$ in the steady-state flow. The rate process theory[13] is applied to the steady flow process, and Eq. (2c), which is very similar to Eq. (1c), is obtained.

(2) Correlation between Dislocation Movement and Grain Boundary Movement. In the deformation of polycrystals, total strain rate $\dot{s}$ is expressed as $\dot{s}=\dot{s}_d+\dot{s}_g$ according to Eq. (3). The reason for this equality is studied in the following. Let us consider two crystallites in contact in a polycrystal. The distance between two planes which pass the center of mass (CM) of crystallite A and that of crystallite B is λ_1. When A shears against B by grain boundary movement, the shear rate $\dot{s}_g$ is expressed by Eq. (2c), where the subscript gj indicates that the attached quantities are those belonging to the jth kind of grain boundary flow units of grain A. That is, $\dot{s}_g$ is the shear rate of the CM of grain A against the plane passing through the CM of grain B.

There are many dislocation slip planes inside grain A, and the shear rate of a dislocation line $\dot{s}_d$ is expressed by Eq. (1c) according to the Ree-Ree-Eyring mechanism.[8] But, λ_1 in this case is the distance between a dislocation slip plane in grain A and the plane including the CM of grain B. That is, $\dot{s}_d$ is the shear rate of the dislocation line under consideration against the CM plane of grain B. Let us assume that all the dislocation slip planes in grain A are all parallel. Then the magnitude of the shear of each shear plane increases as λ_1 increases (grain B is fixed). But the shear rates of these slip planes (amount of shear per unit time/λ_1) are all equal (due to the principle of similar triangle). Now we assume a dislocation slip plane passing through the CM of grain A. Then the shear rate of the hypothetical slip plane can be expressed as $\dot{s}_d$. That is, $\dot{s}_d$ can be considered as the shear rate of the CM of grain A against the plane passing through the CM of grain B. So when grain A shears against grain B by these two different mechanisms (grain boundary movement and dislocation movement), the total shear rate $\dot{s}$ can be expressed as $\dot{s}=\dot{s}_d+\dot{s}_g$, Eq. (3).

For the case of single crystals, λ_1 in Eq. (1c) is the perpendicular distance between two successive dislocation slip planes, and λ has the same meaning of $(m\lambda'/Z)$ in Ree-Ree-Eyring theory.[8]

(3) Molecular Meaning of the Mechanical Models. Finally, we consider the correlation between the mechanical models in *Fig.* 1 and the molecular views mentioned above. The Maxwell model for dislocation movement corresponds to a bad site of a dislocation line held up by a bad site on a slip plane, the release of the dislocation line from the bad site on the slip plane corresponding to the movement of the dashpot of the Maxwell model. A similar statement holds for the Maxwell model for grain boundary movement, i.e., the encounter of a bad site on the surface of grain A with a bad site on the slip plane of grain B corresponds to the Maxwell model for grain boundary movement, and the release of the bad site of grain A from that of grain B represents to the dashpot movement of the Maxwell model. We have applied the rate theory to the release process of a bad site on the flow unit from the bad site of the counter part on the shear plane for both dislocation and grain boundary movements.

APPENDIX 1

In Case 4, the parameters $(\alpha_{d1}, 1/\beta_{d1})$ and $(\alpha_{g2}/X_{g2}, 1/\beta_{g2})$ were determined in the extreme high and low stress ranges, respectively. The contribution due to the GB1 flow units appears over the middle stress range where the contributions due to disln. 1 and GB2 flow units are not negligible. Thus the determination of the parameters $(\alpha_{g1}/X_{g1}$ and $1/\beta_{g1})$, which should be made in the middle stress range, is performed by the following procedure.

(1) $\dot{s}_{d1}$ at a given stress f is calculated from Eq. (1c) by using the parameters $(\alpha_{d1}, 1/\beta_{d1})$ previously determined.

(2) Next, $\dot{s}_{g2}$ can be calculated from the relation $\dot{s}_{g2}=\dot{s}-\dot{s}_{d1}$, and this is, in turn, equal to $\dot{s}_{g2}=\dot{s}_{g1}$ according to Eq. (2b).

(3) $X_{g2}f_{g2}$ is calculated from the relation $\dot{s}_{g2}=(1/\beta_{g2})\sinh[(\alpha_{g2}/X_{g2})X_{g2}f_{g2}]$, which was rewritten from Eq. (2c), by using the known parameters α_{g2}/X_{g2} and $1/\beta_{g2}$.

(4) $X_{g1}f_{g1}$ is obtained from the relation $X_{g1}f_{g1}=f-X_{g2}f_{g2}$ [refer to Eq. (12)].

(5) From the experimental data of $[\dot{s}^{(1)}, f^{(1)}]$ and $[\dot{s}^{(2)}, f^{(2)}]$ at two points, the values, $[\dot{s}^{(1)}{}_{g1}, X_{g1}f_{g1}{}^{(1)}]$ and $[\dot{s}^{(2)}{}_{g1}, X_{g1}f_{g1}{}^{(2)}]$, at these two points are calculated by using the above-mentioned process. By introducing these values to the relation $\dot{s}_{g1}=(1/\beta_{g1})\sinh[(\alpha_{g1}/X_{g1})X_{g1}f_{g1}]$, the parameters $(\alpha_{g1}/X_{g1}, 1/\beta_{g1})$ can be calculated.

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